

# Ethanone, 1-(1,3-dimethyl-1H-indol-2-yl)-

<b>Other names:</b>	Ketone, 1,3-dimethylindol-2-yl methyl 2-Acetyl-1,3-dimethylindole 1,3-Dimethyl-2-acetylindole
<b>Inchi:</b>	InChI=1S/C12H13NO/c1-8-10-6-4-5-7-11(10)13(3)12(8)9(2)14/h4-7H,1-3H3
<b>InchiKey:</b>	KMVJHDBDTPGOGY-UHFFFAOYSA-N
<b>Formula:</b>	C12H13NO
<b>SMILES:</b>	CC(=O)c1c(C)c2ccccc2n1C
<b>Mol. weight [g/mol]:</b>	187.24
<b>CAS:</b>	16244-26-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	2.689		Crippen Method
mcvol	152.570	ml/mol	McGowan Method
rinpol	1811.00		NIST Webbook
rinpol	1852.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16244261&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16244261&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/94-179-0/Ethanone-1-1-3-dimethyl-1H-indol-2-yl.pdf>

Generated by Cheméo on 2024-04-18 00:13:41.433747836 +0000 UTC m=+15688470.354325147.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.